

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.27e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 3.53e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,4-Dichloronaphthalene</div> <div>Measured: 3.38e-05</div> <div>Predicted: 2.77e-03</div>	<div>Image not found</div> <div>2,4,6-Trinitrotoluene</div> <div>Measured: 1.87e-07</div> <div>Predicted: 1.50e-05</div>	<div>Image not found</div> <div>MCPA</div> <div>Measured: 8.25e-05</div> <div>Predicted: 1.19e-06</div>
<div>Image not found</div> <div>Siduron</div> <div>Measured: 1.00e-09</div> <div>Predicted: 2.67e-08</div>		